

L4 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1961:81882 CAPLUS
 DOCUMENT NUMBER: 55:81882
 ORIGINAL REFERENCE NO.: 55:15546b-e
 TITLE: Secosteroids
 INVENTOR(S): Lettre, Hans; Pfirrmann, Rolf
 PATENT ASSIGNEE(S): Farbenfabriken Bayer Akt.-Ges.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1084718		19600707	DE 1958-F26110	19580708

AB 3 β -Hydroxy- or -acyloxy-5,6-secocholestan-5-on-6-al phenylhydrazones or the corresponding derivs. of other 5(6)-unsatd. sterols were reduced, the 3-OH group optionally set free, and the resulting amines substituted or quaternized to give the title compds., useful, as pharmaceuticals. Thus, 1 g. 3 β -acetoxy-5,6-secocholestan-5-on-6-al phenylhydrazone (I) in 150 cc. glacial AcOH was reduced with 6 moles H in the presence of Pt (from 50 mg. PtO₂), the catalyst filtered off, and the filtrate worked up conveniently to give 3 β -acetoxy-5,6-seco-5-hydroxycholestan-6-ammonium acetate (IIa), m. 198° (decomposition). The free amine (II) gave the following derivs.: N-benzoyl derivative m. 262°; benzylidene derivative m. 245-6°. II on saponification with methanolic KOH at room temperature gave 5,6-seco-3 β ,5-dihydroxy-6-amincholestane; benzylidene derivative 231°. I (0.2 g.) reduced by LiAlH₄ in 50 cc. Et₂O gave 5,6-seco-3 β ,5-dihydroxycholestan-6-al phenylhydrazone, m. 203-4° (MeOH), λ 270 m μ , which on catalytical reduction gave amorphous 5,6-seco-3 β ,5-dihydroxy-6-amincholestane. I (1.3 g.) in 100 cc. EtOAc reduced with 1 mole H in the presence of Pt (from 50 mg. PtO₂) gave 3 β -acetoxy-5,6-seco-5-hydroxycholestan-6-al phenylhydrazone, m. 194°, λ 270 m μ , which on further reduction under the same conditions gave II. IIa (1 g.) in 20 cc. 85% HCO₂H heated 2 hrs. with 2 cc. aqueous 40% CH₂O, the mixture concentrated, the residue taken up in dilute NaOH, extracted with Et₂O, the extract washed, dried, and concentrated gave 5,6-seco-3 β ,5-dihydroxy-6-dimethylamincholestane (III), m. 172° (EtOAc); HCl salt m. 280-3° (MeOH-EtOAc). III (0.2 g.) in Et₂O and excess MeI kept 4 weeks at room temperature gave 5,6-seco-3 β ,5-dihydroxycholestan-6-trimethylammonium iodide, m. 194° (EtOAc).

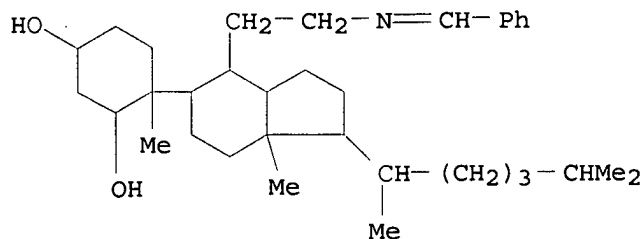
IT 103400-87-9 109214-52-0
 (Derived from data in the 6th Collective Formula Index (1957-1961))

RN 103400-87-9 CAPLUS

CN 1,3-Cyclohexanediol, 4-[4-(2-benzylideneaminoethyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl-5-indanyl]-4-methyl-, acetate (6CI) (CA INDEX NAME)

CM 1

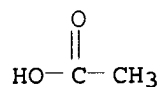
CRN 103400-86-8
 CMF C34 H55 N O2



CM 2

CRN 64-19-7

CMF C2 H4 O2



RN 109214-52-0 CAPLUS

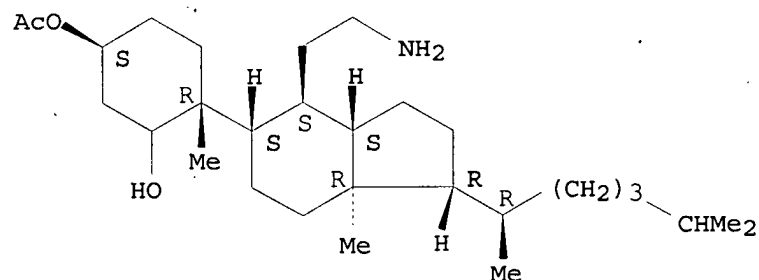
CN 5,6-Secocholestane-3 β ,5-diol, 6-amino-, 3-acetate, compd. with AcOH
(6CI) (CA INDEX NAME)

CM 1

CRN 109214-51-9

CMF C29 H53 N O3

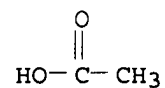
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2

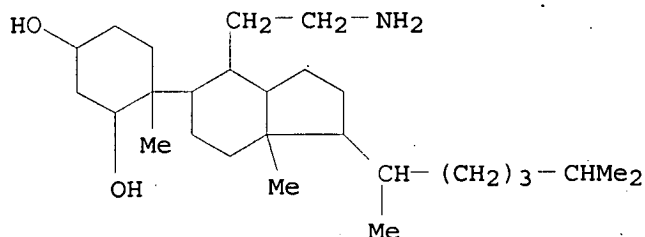


IT 103099-54-3, 1,3-Cyclohexanediol, 4-[4-(2-aminoethyl)-1-(1,5-

dimethylhexyl)hexahydro-7a-methyl-5-indanyl]-4-methyl-
(and derivs.)

RN 103099-54-3 CAPLUS

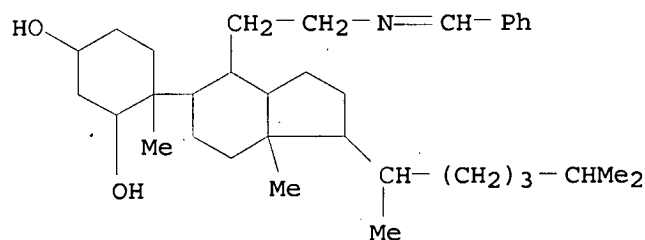
CN 5,6-Secocholestane-3 β ,5-diol, 6-amino- (6CI) (CA INDEX NAME)



IT 103400-86-8P, 1,3-Cyclohexanediol, 4-[4-(2-benzylideneaminoethyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl-5-indanyl]-4-methyl-
105520-54-5P, 5,6-Secocholestane-3 β ,5-diol, 6-dimethylamino-
105520-55-6P, 1,3-Cyclohexanediol, 4-[4-(2-dimethylaminoethyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl-5-indanyl]-4-methyl-, hydrochloride
119300-63-9P, Benzamide, N-[2-[5-(2,4-dihydroxy-1-methylcyclohexyl)-1-(1,5-dimethylhexyl)-hexahydro-7a-methyl-4-indanyl]-ethyl]-, 4-acetate 119300-64-0P, 1,3-Cyclohexanediol, 4-[4-(2-benzylideneaminoethyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl-5-indanyl]-4-methyl-, 1-acetate 122426-28-2P, 5,6-Secocholestane-3 β ,5-diol, 6-dimethylamino-, methiodide
RL: PREP (Preparation)
(preparation of)

RN 103400-86-8 CAPLUS

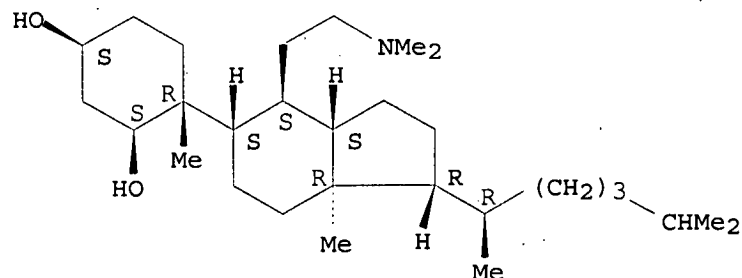
CN 5,6-Secoergostane-1,3-diol, 6-[(phenylmethylene)amino]-, (3 α ,10 α)- (9CI) (CA INDEX NAME)



RN 105520-54-5 CAPLUS

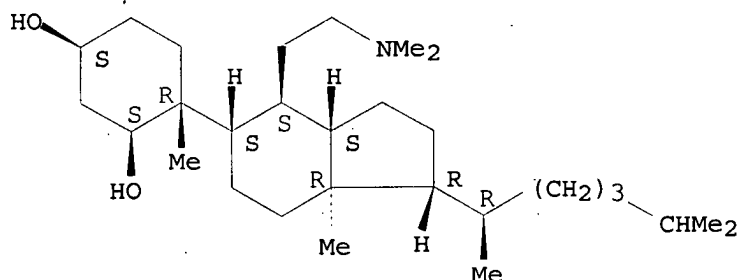
CN 5,6-Secocholestane-3 β ,5 β -diol, 6-dimethylamino- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 105520-55-6 CAPLUS
 CN 5,6-Secocholestane-3 β ,5 β -diol, 6-dimethylamino-, hydrochloride
 (6CI) (CA INDEX NAME)

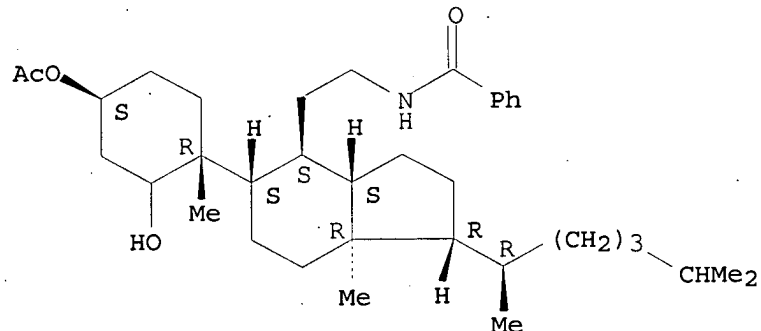
Absolute stereochemistry.



● HCl

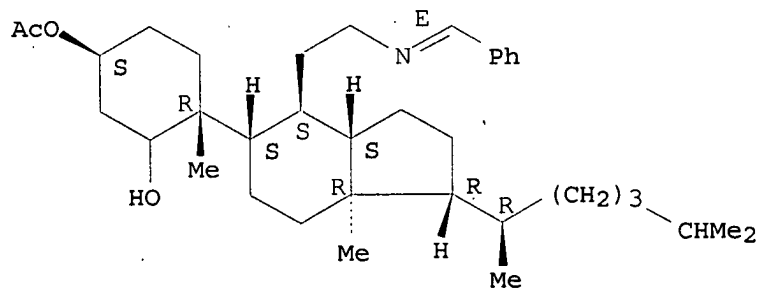
RN 119300-63-9 CAPLUS
 CN 5,6-Secocholestane-3 β ,5-diol, 6-benzamido-, 3-acetate (6CI) (CA
 INDEX NAME)

Absolute stereochemistry.

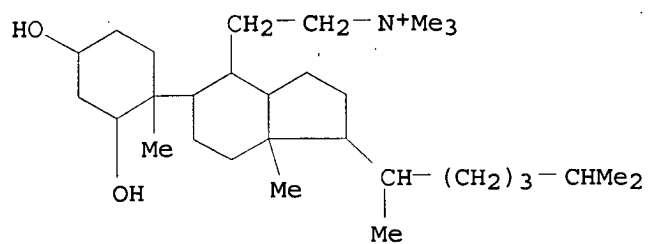


RN 119300-64-0 CAPLUS
 CN 5,6-Secocholestane-3 β ,5-diol, 6-benzylideneamino-, 3-acetate (6CI)
 (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



RN 122426-28-2 CAPLUS

CN 5,6-Secocholestane-3 β ,5-diol, 6-dimethylamino-, methiodide (6CI) (CA
INDEX NAME)● I⁻